



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  
WASHINGTON D.C., 20460

OFFICE OF  
CHEMICAL SAFETY AND  
POLLUTION PREVENTION

**MEMORANDUM**

**DATE:** June 20, 2019

**SUBJECT:** Methods for Assessing Aquatic Exposure to Residue(s) of Concern

**TO:** Environmental Fate and Effects Division (7507P)

**FROM:** Marietta Echeverria, Division Director  
Environmental Fate and Effects Division (7507P)

*Marietta Echeverria*

2019.06.20

09:35:41 -04'00'

Exposure assessments conducted in support of pesticide regulatory decisions typically provide a quantitative analysis of the critical environmental fate and transport properties of the pesticide active ingredient (or parent compound). In some situations, parent compound and or environmental transformation products are also identified as residues of concern. In such situations, exposure assessments include a quantitative or qualitative analysis of the potential exposure and associated risk from these transformation products in most cases the pesticide active ingredient and are identified collectively as residue(s) of concern (ROC). The nature of the stressor evaluated in the risk assessment, including the pesticide active ingredient and environmental transformation products, should always be clearly and concisely described and be based on available data. This memorandum and associated attachments provide guidance and considerations when assessing aquatic exposure to ROC either combined or individually.

Transformation products formed at greater than or equal to 10% of the applied test compound in environmental fate studies are considered a major transformation product and must be identified. The 10% criterion is a general guideline. For example, transformation products approaching concentrations of 10% of the applied test compound are usually identified in the study in addition to transformation products of known toxicological concern that must be quantified per the guidance and identified even when present at less than 10% of the applied test compound. For ecological and human health risk assessments, concern for pesticide transformation products is determined based on the known or anticipated (estimated or assumed) toxicity and potential exposure.

For the human health risk assessment, ROC for drinking water are identified by the Residues of Concern Knowledgebase Subcommittee (ROCKS), which consists of members from the Health Effects Division (HED) and the Environmental Fate and Effects Division (EFED). Documentation in the form of a memorandum is provided by the ROCKS, and contains a list of all ROC, as well as the reasons for considering each individual ROC. The ROCKS memo is expected to be cited in

drinking water assessments (DWA). For ecological risk assessments (ERA), the effects scientist is expected to, in consultation with the fate scientist, identify ROC by taxa. These residues are expected to be clearly identified and the reason for considering each ROC by taxa should be provided in the “Residues of Concern” section of the ERA. The *Guidance for Residues of Concern in Ecological Risk Assessment* (USEPA, 2012) is expected to be consulted as needed to help identify ROC for ecological risk assessments. The EFED ROCKS members can also be consulted.

Once ROC are identified, EFED employs various strategies to estimate exposure to the ROC in aquatic environments; often, this involves considering exposure to multiple ROC. Three of these aquatic exposure modeling methods were presented to a Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) Scientific Advisory Panel (SAP) (USEPA, 2008) on how to estimate exposure to multiple ROC. The three methods presented to the SAP included the Total Residue (TR), Formation and Decline (FD), and the Residue Summation (RS). As presented, the SAP thought the strengths and limitations of the methods were well defined, the methods reflected the current state of the science, and noted that the FD method was the most realistic method of the three. The SAP expressed concern with the temporal occurrence of the ROC assumed in the RS method. While the RS method has been used in risk assessment, upon further investigation recent analysis of this method shows that it does not accurately account for the mass of the ROC over time, as such, should no longer be employed in EFED assessments.

These methods are defined below. Technical guidance for using the TR and FD methods are provided in the attachments and describes why the RS method is no longer considered appropriate for regulatory purposes.

**TR:** This modeling method assumes all ROC have similar physical, chemical, and partitioning characteristics and can be modeled using aquatic exposure models such as the Pesticide in Water Calculator (PWC) (USEPA, 2017) with a combination of parameters from parent or individual ROC. Application rates for the parent pesticide is used to represent the total mass loading of the ROC. This method does not consider temporal occurrence of individual ROC, as the residues are summed at each sampling interval in each of the available environmental fate studies to estimate half-life values and associated modeling input values.

**FD:** This method estimates simultaneous formation and decline rate constants for parent and individual ROC, and the subsequent PWC output includes estimated concentrations of ROC, individually. Application rate adjustments are not needed to account for formation and decline of the transformation products. This method accounts for temporal occurrence of transformation products. However, in order to consider using this method, environmental fate and transport data for each ROC, as well as toxicity for individual ROC are required.

**RS:** This modeling method was historically used to estimate concentrations of ROC individually by summing the time series concentration data to estimate combined exposure concentrations of the ROC. Application rates for individual ROC were

developed based on the molecular weight ratios of individual ROC to parent, and the normalized maximum percentage of transformation product observed in the various environmental fate studies. This method required environmental fate data for each ROC.

While this document focuses on the three methods presented to the SAP, there may be other appropriate modeling methods in some limited situations. For example, an individual ROC may be modeled alone using ROC-specific data and adjusting the application rate based on the molecular weight difference as well as the stoichiometry. When alternative modeling methods are utilized, the application rate should not be derived using the normalization method employed in the RS method.

This memorandum and associated technical guidance is intended to provide EFED staff assistance on how to consider ROC for both ERA and DWA using these methods, and considers comments received from the SAP. In general, staff should use a tiered approach to consider exposure to ROC. While not necessarily more conservative, the first tier is the TR method, as it requires the least amount of data and resources to complete. Historically, the TR method has been employed across EFED and one goal of this memo is to ensure it is used consistently. The TR method can be used to assess the potential exposure to ROC with differing toxicity if the resulting exposure estimates are compared to the lowest toxicity endpoint of all the ROC. The TR method can be refined using the FD method when data are available to support the analysis, and FD is most appropriate to use when the ROC have different mechanisms of toxicity and differences in environmental fate and transport.

Attached to this memorandum are technical guidance's for completing aquatic modeling for ROC using the TR method (**ATTACHMENT 1**) and considerations for utilizing the FD method (**ATTACHMENT 2**) in quantitative pesticide aquatic exposure assessments. The FD method can provide more confidence in estimates and account for differing toxicity as well as environmental fate and transport differences. There are a number of scientifically robust tools available for evaluation of FD; however, there is no preferred tool. Refinement of the TR method using the FD method (or any other method) should be done consistent with the considerations outlined in the attached technical guidance and in consultation with the senior staff. The Pesticide Fate and Transport Technical Team (PFTTT) in addition to the ROC team (acknowledged below) can be consulted. Assessments conducted using the FD method should be shared with the PFTTT to build a repository of example assessments for reference and to support the development of specific technical guidance for the FD method. Finally, **ATTACHMENT 3** provides a case study for why the RS method should not be used in pesticide exposure assessments. For additional guidance, consult the PFTTT or the EFED science advisors and senior scientists.

#### References

USEPA, 2008. Methods for Assessing Ecological Risks of Pesticides with Persistent, Bioaccumulative and Toxic Characteristics. FIFRA Scientific Advisory Panel. October 28-31, 2008.

USEPA, 2012. Guidance for Residues of Concern in Ecological Risk Assessment, USEPA, December 20, 2012.

USEPA, 2017. The Pesticide Water Calculator. <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment>

#### Acknowledgements

Rochelle F. H. Bohaty, PhD  
Mark Corbin, MS  
Sarah C. Hafner, PhD  
Jessica L. O. Joyce, MS  
Kurt Pluntke, MS  
Mohammed Ruhman, PhD  
Henry Nelson, PhD

R. David Jones, PhD  
William P. Eckel, PhD  
James A. Hetrick, PhD  
Nelson Thurman, MS  
Steve P. Wentz, PhD  
Dirk F. Young, PhD

#### Attachments

ATTACHMENT 1 - Assessing Exposure to Residues of Concern Using the Total Residue Method  
ATTACHMENT 2 - Formation Decline Considerations  
ATTACHMENT 3 - A Case Study for Not Using Residue Summation in Quantitative Exposure Assessments

## **ATTACHMENT 1**

### **Assessing Exposure to Residues of Concern Using the Total Residue Method**

This attachment provides guidance for using the total residue (TR) method for risk assessment purposes. If multiple residues of concern (ROC) are identified, the Environmental Fate and Effects Division (EFED) may employ various modeling strategies to estimate exposure to ROC concentrations in aquatic environments. Of the approaches for modeling ROC, the TR method is the most commonly used and the simplest to implement. The TR method is used to derive estimated drinking water concentrations (EDWC) and estimated environmental concentrations (EEC) for the combined ROC using aquatic models such as Pesticide Water Calculator (PWC) (USEPA, 2017). This modeling method assumes that all ROC have similar physical, chemical, and partitioning characteristics to each other. This modeling approach does not directly consider temporal occurrence (*i.e.*, formation timing) of transformation products. This method was present to and received positive feedback from the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA) Scientific Advisory Panel (SAP) (USEPA, 2008).

This method is best employed for residues with similar or the same toxicity as it assumes that all the constituents have the same toxicity and/or mode of action. However, the TR method can be used if the toxicity differs between the ROC, if the risk assessment is conducted considering the toxicity profile of each of the individual ROC. For example, if the toxicity of the most toxic ROC is compared to the TR exposure estimates that does not result in an exposure concern, there is high confidence there is no risk.

If this method results in an exposure concern, there could be risk, or it may be the result of overestimating exposure based on the assumed environmental fate parameters or toxicity. If this occurs, characterization of the representation of the model inputs and toxicity related to the ROC is necessary. In addition, refining the exposure estimates using the Formation Decline (FD) method (**ATTACHMENT 2**) should be considered in light of the available data. Senior staff as well as the Pesticide Fate and Transport Technical Team (PFTTT) may be consulted.

The TR method incorporates all scientifically available data deemed robust enough for use in exposure assessment to conservatively estimate ROC exposure estimates resulting from the use being assessed. The method involves a two-step process: (1) estimation of fate/transport parameters necessary for modeling of the ROC, and (2) execution of model simulations for various scenarios (based on use patterns) to obtain ROC exposure estimates. This process is no different than the standard process employed in aquatic exposure assessments; however, the model input values no longer reflect pesticide active ingredient or parent compound-only values, but rather reflect a combination of all the ROC.).

Application rates for the parent pesticide are used to represent the total mass loading of the ROC. TR model input parameters are derived by examining relevant environmental fate studies (hydrolysis, aqueous photolysis, aerobic soil metabolism, etc.) and calculating:

1. The sum of the concentrations of the ROC (parent pesticide and/or the transformation product(s) determined to be ROC) at each sampling interval present in each study. Refer to **Table 1.2**.
2. The rate constant and the corresponding half-life value for the ROC for each study based on the total residue calculated above. Refer to **Figure 1.1**.
3. The modeling input parameters following the model input parameter guidance (USEPA, 2009), and **Table 1.1.**, below.

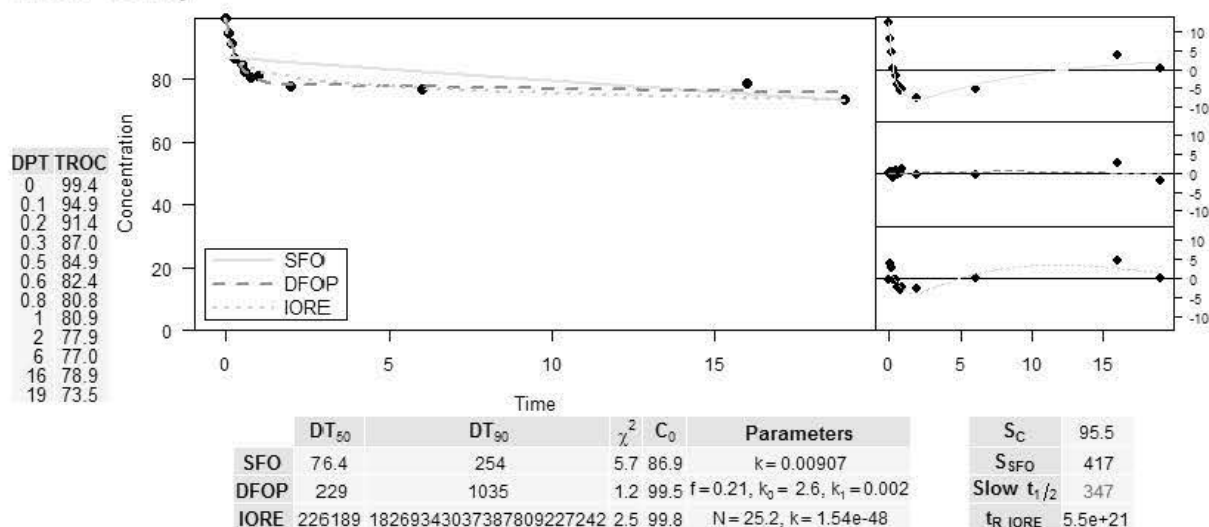
**Table 1.1. Basis for Selecting Physical-chemical and Environmental Fate Modeling Input Parameters for Residues of Concern Using the Total Residue Method**

Input Parameter (Unit)	Basis for Selection
Sorption Coefficient ( $K_d$ or $K_{oc}$ ) (mL/g)	Mean $K_{oc}$ or $K_d$ of the most mobile compound (parent or ROC)
Water Column Metabolism (Aerobic Aquatic Metabolism) half-life ( $t_{1/2}$ in days)	Re-calculate half-life values for the total ROC by summing the concentration of all ROC at each sampling interval, and regressing the summed concentration values with time to calculate a new half-life for each study test system (see <b>Table 1.2</b> and <b>Figure 1</b> ) (USEPA, 2015). Then calculate model input parameter per input parameter guidance (USEPA, 2009).
Benthic Metabolism (Anaerobic Aquatic Metabolism) Half-life ( $t_{1/2}$ in days)	
Aqueous Photolysis Half-life ( $t_{1/2}$ in days @ pH 7)	
Hydrolysis Half-life ( $t_{1/2}$ in days)	
Soil (Aerobic Soil Metabolism) Half-life ( $t_{1/2}$ in days)	
Molecular Weight (M Wt.) g/mole	Value for parent compound
Henry's constant ( $\text{atm}\cdot\text{m}^3\text{mol}^{-1}$ @ 25 °C)	Most conservative value considering data for each of the ROC ( <i>i.e.</i> , the lowest value)
Vapor Pressure (torr @ 25 °C)	Most conservative value considering data for each of the ROC ( <i>i.e.</i> , the lowest value)
Solubility (in Water) (mg/L)	Most conservative value considering data for each of the ROC ( <i>i.e.</i> , the highest value)
Application rate, date, frequency, intervals, chemical application method, efficiency and Spray Drift	Values used for the pesticide from the label and as per the model input parameter guidance documents (USEPA, 2012; USEPA 2013)

**Table 1.2. Case Study: Transformation of Parent Pesticide to Residues of Concern 1 and 2**

Days Post-Treatment	Parent	ROC 1	ROC 2	Total (Parent + ROC 1 and ROC 2)
	% Applied Radioactivity			
0	99.4	0	0	99.4
0.1	77.2	15.9	1.8	94.9
0.2	58.9	26.7	5.8	91.4
0.3	43.1	35.9	8	87
0.5	30.9	40.8	13.2	84.9
0.6	22.4	42.8	17.2	82.4
0.8	11.8	44.2	24.8	80.8
1	7.1	44.4	29.4	80.9
2	0	26	51.9	77.9
6	0	2.1	74.9	77
16	0	0	78.9	78.9
19	0	0	73.5	73.5

## Case Study



**Figure 1.1. Case Study: Kinetic Analysis of Parent Pesticide to Residue of Concern 1 and 2**

**Table 1.1** provides an explanation for selecting a ROC model input value for each physical-chemical and environmental fate modeling input parameter for aquatic modeling. When there are no physical-chemical or environmental fate data available for the identified transformation products, input values are assumed to be equivalent to the parent value, as well as if the value cannot be reasonably estimated using a tool such as EPI Suite (USEPA, 2012). For example, if the vapor pressure is not available for a transformation product, the input value for the ROC is assumed to be equal to the parent value. If data are available for both parent compound and transformation products, and the data cannot be combined (*e.g.*, mobility or solubility data),

the most conservative mean value of the parent or ROC should be used. If the approach presented in **Table 1.1** requires refinement, alternative input parameters may be considered in light of, temporal occurrence, properties of residues present in greatest amount, etc. The justification for selecting each model input value including deviations from the standard approach below should be clearly reported in the associated pesticides exposure assessment.

## References

- USEPA, 2008. Methods for Assessing Ecological Risks of Pesticides with Persistent, Bioaccumulative and Toxic Characteristics. FIFRA Scientific Advisory Panel. October 28-31, 2008. [http://www.epa.gov/scipoly/sap/meetings/2008/102808\\_mtg.htm](http://www.epa.gov/scipoly/sap/meetings/2008/102808_mtg.htm).
- USEPA, 2009. Guidance for Selecting Input Parameters in Modeling the Environmental Fate and Transport of Pesticides, Version 2.1.
- USEPA, 2012a. Guidance on Modeling Using AgDRIFT/AgDISP in Ecological Risk Assessment in the Environmental Fate Effects Division.
- USEPA, 2012b. EPI Suite. <https://www.epa.gov/tsca-screening-tools/epi-suite-tm-estimation-program-interface>.
- USEPA, 2013. Guidance on Modeling Offsite Deposition of Pesticides Via Spray Drift for Ecological and Drinking Water Assessment.
- USEPA, 2014. Standard Operating Procedure for Using the NAFTA Guidance to Calculate Representative Half-life Values and Characterizing Pesticide Degradation.
- USEPA, 2015. Release of Update to the Standard Operating Procedure for Calculating Degradation Kinetics in Environmental Media.
- USEPA, 2017. The Pesticide Water Calculator. <https://www.epa.gov/pesticide-science-and-assessing-pesticide-risks/models-pesticide-risk-assessment>.

## ATTACHMENT 2

### Formation Decline Considerations

This document provides guiding principles and considerations for using the Formation Decline (FD) method for risk assessment purposes. The FD method is an explicit method for quantitative exposure assessment when multiple residues of concern (ROC) are identified and environmental fate data are available to support the analysis. This method is most commonly used to generate exposure concentrations from the Pesticide in Water Calculator (PWC) for each ROC; however, other aquatic modeling exposure tools may be used.

The FD method requires estimation of the molar formation and decline ratios (MFDR<sup>1</sup>) for parent compound and transformation products (*i.e.*, ROC). There are various methods to determine the MFDR for parent and degradation products including stoichiometry, as well as a simultaneous curve fitting approach across parent and transformation products. The MFDR estimation is suited for single first order degradation kinetics. In addition to laboratory study data, other environmental fate data for the transformation products are necessary to employ the FD method (*e.g.*, soil mobility data). Several guiding principles are listed below for consideration when using the FD method. The Pesticide Fate and Transport Technical Team (PFTTT) should be consulted when using the FD method for assistance in selecting and using suitable tools for estimating the simultaneous formation and decline rate constants for parent and transformation products.

#### Guiding Principles

1. The FD method is routinely applied as a refinement following use of the Total Residue (TR) method (**ATTACHMENT 1**).
2. The FD method is a more effective refinement when the ROC differ in toxicity (*i.e.*, the assumption of equal toxicity does not hold) or where the residues greatly differ in relative mobility (based on  $K_{oc}$  or  $K_d$  values). In other instances, the refinement may make little difference in the exposure estimates.
3. Single first order (SFO) kinetics data are required for parameterizing PWC. Environmental fate data need to be available that track the decline of the parent compound as well as the formation and decline of all transformation products

---

<sup>1</sup> MFDR is the ratio of moles of the transformation product produced to moles of parent compound transformed. For example, if one parent molecule breaks down and produces one molecule of the transformation product, then the ratio is 1. If the parent transforms to form 2 molecules of the transformation product, then the ratio is 2. If the process does not produce the transformation product of interest, then the ratio is zero. Empirical data for the rates of formation and decline can be used to derive the MFDR for situations where there is a loss of the parent compound to another transformation pathway or sorption. For example, often there are competing chemical transformation pathways that result in the formation of two different transformation products from the same parent compound that do not transform to become the other compound.

considered in the FD method. The quality of the available data for each chemical considered a ROC needs to be considered prior to employing the FD method.

4. The PWC can only be used with a parent → daughter(s) → granddaughter(s) transformation pathway. If the transformation pathway is more complicated than this, the data must be adapted to parent → daughter(s) → granddaughter(s).
5. Generally, the number of data points from each environmental fate study should be five or more as required in study guidelines.
6. Various tools exist that can be used to estimate the simultaneous formation and decline rate ratios for parent and transformation products; however, it should be noted that most available tools rely on use of SFO kinetics. As such, if a SFO-based tool is used for assessing data that do not follow SFO kinetics (*i.e.*, biphasic), the implications of force fitting a SFO model to the data needs to be characterized in the associated exposure assessment. This includes characterization of the parent compound half-life value derived from North American Free Trade Agreement (NAFTA) kinetics guidance (USEPA, 2015) and the value derived with the SFO-based formation decline tool.
7. Formation and decline rates are required for calculating the molar formation and decline ratios needed for modeling exposure (EEC and EDWC) using for example, the PWC.
8. Data from multiple soils should not be combined (*i.e.*, combined to generate a model input value used in the PWC). As such, estimation of simultaneous formation and degradation rate constants for parent compound and transformation products should be conducted for all available data, one soil at a time, and a bounding approach should be employed for quantitative exposure estimates. That is, formation and decline rates from different soils can be used to calculate upper- and lower-bound exposure concentrations for the parent compound and associated transformation products (*e.g.*, fastest parent transformation rate and the slowest rate of parent transformation).
9. Estimated values [*e.g.*, EPI Suite (USEPA, 2012)] may be used; however, the confidence in the estimated values should be characterized in the assessment.

#### References

USEPA, 2015. Release of Update to the Standard Operating Procedure for Calculating Degradation Kinetics in Environmental Media.

### ATTACHMENT 3

#### A Case Study for Not Using the Residue Summation Method in Exposure Assessments

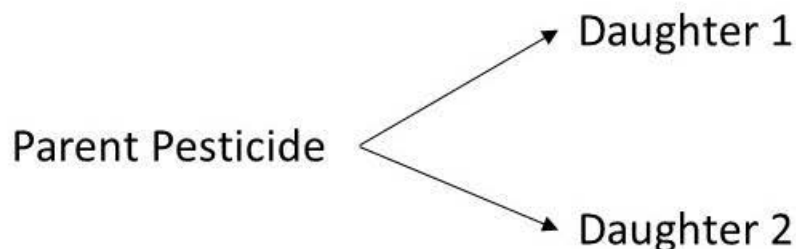
The Residue Summation (RS) method was originally proposed to derive pesticide exposure concentrations for multiple residues of concern (ROC). This method has been used in risk assessments; however, **the RS method should no longer be used in aquatic exposure assessments used for regulatory purposes.** This attachment is provided to document historic discussions and subsequent decisions on the utility of the RS method for regulatory purposes.

The RS methodology was presented to the Federal Insecticide, Fungicide, and Rodenticide Act Scientific Advisory Panel (SAP) (USEPA, 2008). In summary, the method derives an application rate for each of the individual ROC by normalization, then each ROC is modeled separately using available residue specific environmental fate and transport data, and finally, the time series data (daily concentration data) for each individual ROC is summed for each day. From this new time series of concentrations, new exposure estimates (*e.g.*, 1-in-10 year 1-day average, 1-in-10 year 365-day average, of simulation average (*i.e.*, 30-year average) concentrations are derived.

Since the SAP, the RS method has been used in risk assessments. However, upon further consideration and analysis, EFED has determined that the RS approach should no longer be used for risk assessment purposes, including EDWCs and EECs. The reasons for this include:

1. The RS method inaccurately accounts for pesticide mass in the system, both through normalization of the parent compound application rate, and by disregarding transformation product formation.
2. The RS method does not accurately account for the temporal occurrence of parent and transformation products. This can result in underestimating the potential exposure to ROC.

The case study presented below illustrates the shortcomings of the RS method by examining a pesticide transforming to two different compounds concurrently, based on empirical transformation data (see **Figure 3.1**). The parent pesticide as well as both transformation products, Daughter 1 and Daughter 2, have been identified as ROC. The study results are presented in **Table 3.1** as well as **Figure 3.2**.

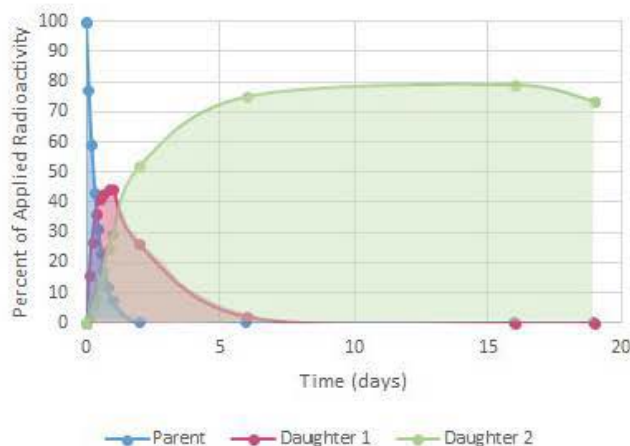


**Figure 3.1. Case Study: Transformation Pathway for RS Case Study**

**Table 3.1. Case Study: Transformation of Parent Pesticide to Daughter 1 and 2**

Days Post-Treatment	Parent	Daughter 1	Daughter 2	Total (Parent + Daughters)
	% Applied Radioactivity			
0	99.4*	0	0	99.4
0.1	77.2	15.9	1.8	94.9
0.2	58.9	26.7	5.8	91.4
0.3	43.1	35.9	8	87
0.5	30.9	40.8	13.2	84.9
0.6	22.4	42.8	17.2	82.4
0.8	11.8	44.2	24.8	80.8
1	7.1	44.4*	29.4	80.9
2	0	26	51.9	77.9
6	0	2.1	74.9	77
16	0	0	78.9*	78.9
19	0	0	73.5	73.5

\* indicates date of highest formation



**Figure 3.2. Case Study: Transformation Profile of Parent Pesticide to Daughter 1 and 2**

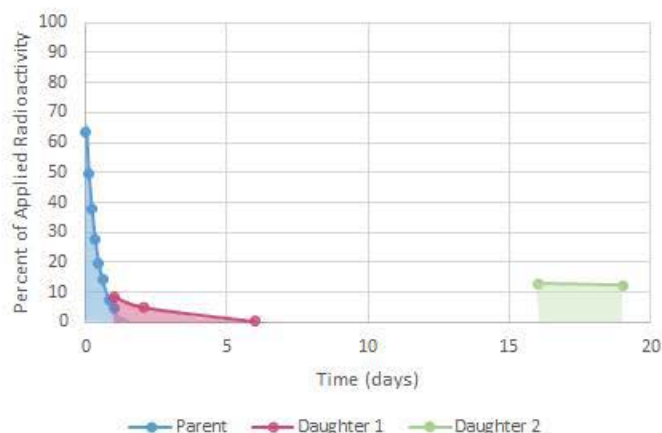
The parent pesticide is assumed to be applied at a rate of 1 kg/ha, and the molecular weight is 300 g/mol. The molecular weights for each ROC (Daughters 1 and Daughter 2) are assumed to be 200 g/mol and 100 g/mol, respectively. The data are transformed into an adjusted application rate for each ROC (parent compound and transformation product), following the RS method. **Table 3.2** includes the necessary calculations to determine the application rate for modeling each ROC individually.

**Table 3.2 Case Study: Residue Summation Calculation for Modeled Application Rates**

Chemical	Maximum Percent Applied Radioactivity Observed		Application Rate (kg/ha)	Molecular Weight Ratio	Adjusted Modeled Application Rate (kg/ha)	Adjusted Percent of Modeled Application Rate
	Observed	Normalized				
Parent	99.4	44.6	0.45	1	0.45	64.1
Daughter 1	44.4	19.9	0.20	0.67 <sup>a</sup>	0.13	19.2
Daughter 2	78.9	35.4	0.35	0.33 <sup>b</sup>	0.12	16.8
Total	<b>222.7</b>	<b>100</b>	<b>1.0</b>	---	<b>0.70</b>	---
a. 200 g/mol / 300 g/mol = 0.67						
b. 100 g/mol / 300 g/mol = 0.33						

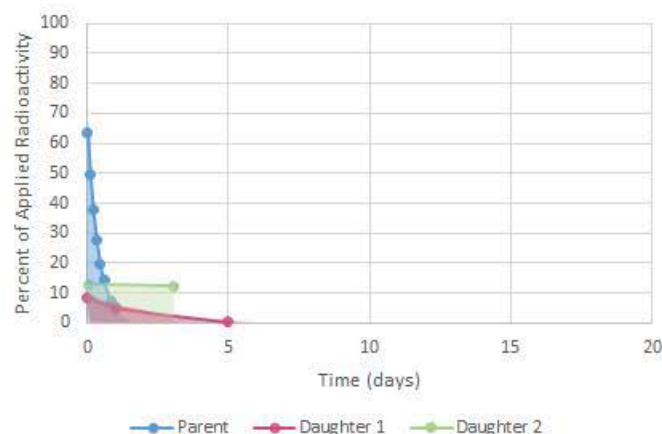
The first shortcoming outlined above is illustrated in the adjusted modeled application rate for parent in **Table 3.2**. While the parent pesticide is labeled at an application rate of 1 kg/ha, the adjusted modeled application rate using the RS method accounts for only 0.45 kg/ha of parent. Parent pesticide is underestimated by the adjusted application rate derived from a normalized concentration based on maximum observed concentration for each of the ROC. This ultimately underestimates the parent pesticide loading by assuming that the daughters are applied instead of parent pesticide, rather than forming from the parent. These calculations also assume that parent pesticide and the modeled ROC account for total applied mass, though peak formation may not be captured by the observed samples, and other residues (not of concern) may also be formed. This is demonstrated in **Table 3.1**, which shows that these residues (parent, daughter 1, and daughter 2) account for only 73.5% of the applied radioactivity by the end of the study. For these reasons, exposure to parent pesticide will not be captured in exposure estimates. Moreover, the potential exposure to the transformation products may also be underestimated as the maximum observed concentration of the transformation products in the study may not be the true maximum concentration in the environment.

**Figure 3.3** depicts the laboratory study adjusted results following the normalization procedure described above for the RS method with respect to time. This figure describes when the maximum concentrations were observed for each ROC (and not the application date). The percent of applied radioactivity is adjusted for the percent of mass applied (**Table 3.2**) for each residue.



**Figure 3.3. Case Study: Normalization of Residues Based on Residue Summation Approach for a Hypothetical Study**

**Figure 3.3** represents a modeling situation where the application date of each ROC is offset to reflect the date of when the maximum concentration was observed; however, the RS method recommends modeling application of the parent pesticide and the two daughters on the same date. The impact of this assumption for this hypothetical study is presented in **Figure 3.4**. This enhances the inaccuracies in the temporal occurrence of the transformation products.



**Figure 3.4. Case Study: Effective Modeled Chemical Loading Based on Residue Summation Approach for One Laboratory Study**

The RS method shortcomings are best illustrated by comparing **Figure 3.2** to **Figure 3.4**. The comparison between the figures shows both the underestimation of pesticide loading, as well as the inaccuracies in the temporal occurrence of transformation products, which leads to compounding inaccuracies in the assumed persistence and transport of residues if assumed when conducting aquatic exposure modeling. One suggestion to address the temporal inaccuracy is to offset the application date to correspond to the date of maximum observed concentration in the study as shown in **Figure 3.3**; however, this does not account for the formation of the transformation products overtime or total parent pesticide mass applied. As discussed previously, the inherent assumptions of the RS method, and the resulting mass

applied relative to the overall mass of ROC present in the environment is not accurately or reasonably reflected. As such, use of the RS method for aquatic exposure modeling is not recommended for regulatory purposes.

#### References

USEPA, 2008. Methods for Assessing Ecological Risks of Pesticides with Persistent, Bioaccumulative and Toxic Characteristics. FIFRA Scientific Advisory Panel. October 28-31, 2008. [http://www.epa.gov/scipoly/sap/meetings/2008/102808\\_mtg.htm](http://www.epa.gov/scipoly/sap/meetings/2008/102808_mtg.htm).